Focus Report

New Chemicals Program

PMN Number: **P-04-0463**

Focus Date:	04/12/2004 01:00:00 AM	Report Status:	Completed
Consolidated Set:			
Focus Chair:	A. Binder	Contractor:	HAH

I. Notice Information

Submitter:	WSP Chemicals & Technology, LLC	CAS Number:	
Chemical Name:	2-PROPENOIC ACID, 2-METHYL-, 2-(DIMETHYLAMINO)ETHYL ESTER, HOMOPOLYMER, COMPD. WITH 1-BROMOHEXADECANE*		
Use:	Oilfield down hole applications		
Other Uses:	Awaiting ISIS Entry		
PV-Max:	11,000 Kg/yr		
Manufacture:	X	Import:	

Production Volume other information:

II. SAT Results

(1) **Health Rating:** 1-2 **Eco Rating:** 3 **Comments:** ;

Additional SAT information:

Occupational: NR **Non-Occupational:** - **Environmental:**

(1) **PBT:**			**Comments:**
Awaiting Fate Entry	Awaiting Fate Entry	Awaiting Human Health Entry	Awaiting Fate Entry
Awaiting Fate Entry	Awaiting Fate Entry	Awaiting Human Health Entry	Awaiting Fate Entry
Awaiting Fate Entry	Awaiting Fate Entry	Awaiting Human Health Entry	Awaiting Fate Entry

III. OTHER FACTORS

Categories:

Health Chemical Category:

Ecotox SAR and TSCA New Chemical Category: ; Polycationic Polymers,

Related Cases/Regulatory History:

Health related Cases:

Ecotox Related Cases:

Regulatory History: [redacted]

MSDS/Label Information:

MSDS: No

Exposure Based Information:

Exposure Based Review:

Exposure Based Review (Eco):

Exposure Based Review (Non Occupatuional):

Exposure Based Review (Health):

Exposure Based (Occupational): No

Exposure Based (Environmental):

IV. Summary of SAT Assessment

Legacy SAT assessment: CASE NUMBER: P04-0463

FATE: MW<100 000 with <1% <1000 and <1% <500 with amine FGEW = 157 = 8.9% amine-N (worst case) and <5% Br solid with mp = unk °C (P)
S = complete (MSDS), fully soluble (PMN), dispersible at pH 7 (RAD)
vp < 1.0E-6 mm Hg or torr at 25 °C (P)
bp > 500 °C (P)
H < 1.0E-8 (P)
log Koc > 4.5 (P)
log fish BCF = 0.50 (P)
POTW removal = 90 to 99% via sorption
time for complete ultimate aerobic biodegradation > months
sorption to soils and sediments = very strong
PBT Potential: P3B1T1

HEALTH: Absorption nil all routes based on physical/chemical properties;

concern for lung overload based on MW and cationic binding with lung membranes based on N FGEW = 157;
concern for irritation to mucous membranes and eyes based on amines;
concerns for the Br salt are liver toxicity and neurotoxicity but the Br salt is less than 5% of PMN substance;

low to moderate concern for toxicity;

ECOTOX: Predicted (P) and measured (M) toxicity values in mg/L (ppm) are:
fish 96-h LC50 = 0.280 P TOC 2
daphnid 48-h LC50 = 0.100 P TOC 2
green algal 96-h EC50 = 0.040 P TOC 2
fish chronic value = 0.020 P TOC 2
daphnid ChV = 0.007 P TOC 2
algal ChV = 0.020 P TOC 2
Predictions are based on SARs for polycationic polymers with 8.9% amine-N; SAR chemical class = polymer-cationic-8.9% amine-N; MW>100 000 with <1% <1000 and <1% <500; pH7; effective concentrations based on 100% active ingredients and nominal concentrations; hardness <150.0 mg/L as CaCO3; and TOC <2.0 mg/L;
high concern for acute toxicity in water with TOC<2.0 mg/L;
mitigation of toxicity expected in the presence of 10 mg TOC/L, i.e., >= 100 times;
low concern for environmental risk at TOC = 10 mg/L;
assessment factor = 10.0
concern concentration >= 1.0 mg/L (ppm) with mitigation due to 10 mg TOC/L;

Fate:

Fate Summary:

Health:

Health Summary:

Ecotox:

Ecotox Values:
Fish 96-h LC50:
Daphnid 48-h LC50:
Green algal 96-h EC50:
Fish Chronic Value:
Daphnid ChV:
Algal ChV:

Ecotox Factors:

Assessment Factor:
Concern Concentration:
- Acute Value
Concern Concentration:

- Chronic Value

Legacy summary of eposures and releases:

V. Summary of Exposures/Releases

Engineering Summary:

Exposures/Releases			
Scenario			
Sites			
Media			
Descriptor A			
Quantity A (kg/site/day)			
Frequency A (day/year)			
Descriptor B			
Quantity B (kg/site/day)			
Frequency B (day/year)			
From			
Workers			
Exposure Type			

VI. Focus Decision and Rationale

Regulatory Actions

Regulatory Decision: Drop Decision Date: 04/12/2004

Type of Decision:

Rationale: P04-0463 was dropped from further review. Potential risks to human health were addressed by negligible inhalation exposures. Although concerns were high, potential risks to the environment were low based on no expected releases to water. This was a CEB D3 Drop.

P2 Rec Comments:

Testing:

Final Recommended:

Health:

Eco:

Fate:

Other:

[redacted]

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Case #: P-04-0463	**DCN:**
SAT Date: 4/2/2004	**SAT Chair:** V. Nabholz

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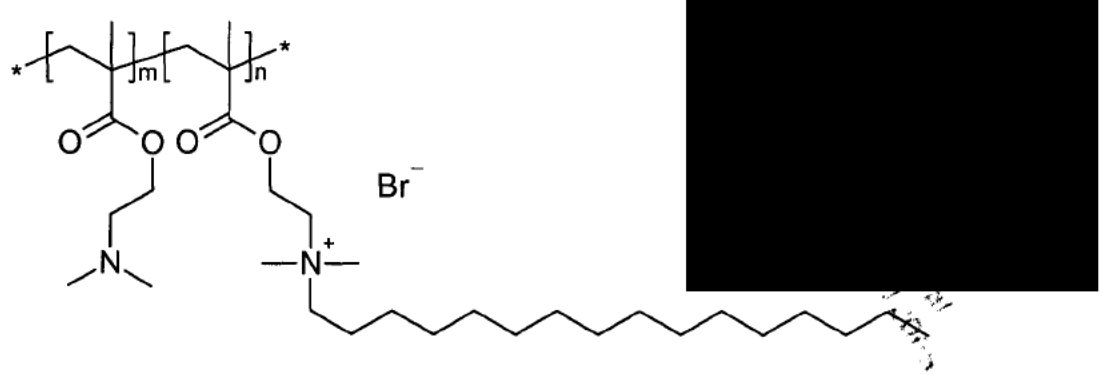
Submitter: WSP Chemicals and Technology, LLC

Chemical Name:

2-Propenoic acid, 2-methyl-, 2-(dimethylamino)ethyl ester, homopolymer, compd. with 1-bromohexadecane

CAS RN:	**Trade Name:**
88677-76-3	HPT-1; FDP-W658

Structure



[redacted]

Molecular Formula: $C_{32}H_{63}BrN_2O_4$

Molecular Wt. 100000	**WT%<500:** 0.50	**WT%<1000:**	0.50
MP:	**BP:**	**Eq. Wt:**	
H2O Sol (g/L): <0.000001	**V.P.**	<0.000001	
Max. Prod. Volume (kg/yr): 11000	**Physical State:**	Solid	

USE:

Thickener used in oil-field down hole application.
Anal[redacted] and [redacted] are used as oil-field production aids. They increase the ratio of crude oil to produced water. They are injected into the underground oil-producing formation where they adhere to the rock. The presence of the polymers in the rock fissures allow the oil to pass, but retard the passage of water. This improves the efficiency of the oil well and reduces the amount of waste water that must be separated and re-injected underground.

Related Case Numbers	Case Role	Related Case Numbers	Case Role

Focus **Date:** APR 12 2004 **Results:** DROP

STRUCTURE ACTIVITY TEAM REPORT 02 April 2004 [redacted]

CASE NUMBER: **P04-0463**

RELATED CASES: [redacted] [redacted]

CONCLUSIONS/DISCUSSIONS

TYPE OF CONCERN:	HEALTH	ECOTOX
LEVEL:	1-2	3

KEYWORDS: LUNG, IRR-E,MM, AQUATOX-A,C

SUMMARY OF ASSESSMENT:

FATE: MW<100 000 with <1% <1000 and <1% <500 with amine FGEW = 157 = 8.9% amine-N (worst case) and <5% Br
solid with mp = unk °C (P)
S = complete (MSDS), fully soluble (PMN), dispersible at pH 7 (RAD)
vp < 1.0E-6 mm Hg or torr at 25 °C (P)
bp > 500 °C (P)
H < 1.0E-8 (P)
log Koc > 4.5 (P)
log fish BCF = 0.50 (P)
POTW removal = 90 to 99% via sorption
time for complete ultimate aerobic biodegradation > months
sorption to soils and sediments = very strong
PBT Potential: P3B1T1
*CEB FATE: migration to ground water = negligible

HEALTH: Absorption nil all routes based on physical/chemical properties;

concern for lung overload based on MW and cationic binding with lung membranes based on N FGEW = 157;
concern for irritation to mucous membranes and eyes based on amines;
concerns for the Br salt are liver toxicity and neurotoxicity but the Br salt is less than 5% of PMN substance;

low to moderate concern for toxicity;
*CEB HEALTH: Exposures to humans: inhalation

ECOTOX: Predicted (P) and measured (M) toxicity values in mg/L (ppm) are:

fish 96-h LC50	=	0.280 P TOC 2
daphnid 48-h LC50	=	0.100 P TOC 2
green algal 96-h EC50	=	0.040 P TOC 2
fish chronic value	=	0.020 P TOC 2
daphnid ChV	=	0.007 P TOC 2
algal ChV	=	0.020 P TOC 2

Predictions are based on SARs for polycationic polymers with 8.9%

amine-N; SAR chemical class = polymer-cationic-8.9% amine-N; MW>100 000 with <1% <1000 and <1% <500; pH7; effective concentrations based on 100% active ingredients and nominal concentrations; hardness <150.0 mg/L as CaCO3; and TOC <2.0 mg/L;
high concern for acute toxicity in water with TOC<2.0 mg/L;
mitigation of toxicity expected in the presence of 10 mg TOC/L, i.e., >= 100 times;
low concern for environmental risk at TOC = 10 mg/L;
assessment factor = 10.0
concern concentration >= 1.0 mg/L (ppm) with mitigation due to 10 mg TOC/L;
*CEB ECOTOX: No releases to water

SAT Co-chair: Vince Nabholz, 564.8909

GTOX Report

PMN No. P-04-0463 | CAS No. 88677-76-3 | Rcvd: 03/24/04 | OECD Incomplet | ID: Rec# 5 : 122

S/A: S | Name of Analog: | Reviewer: NSH

		with activation	without activation	Positive Strains
Salmonella Assay:		☐	☐	
Chromosomal Aberration	CHO:	☐	☐	
	CHL:	☐	☐	
	V79:	☐	☐	
E. coli Reverse Mutation:		☐	☐	
Mouse Micronucleus Assay:	Route:		☐	
Rat Hepatocytes Unscheduled DNA Synthesis:			☐	

Other GTOX Results

Comments

ECOTOX: ☐

Fate:

WS/Log P: Fully soluble @ 25 C, p.22 (complete, MSDS, p.15).

NCSAB SAT REPORT

[redacted]

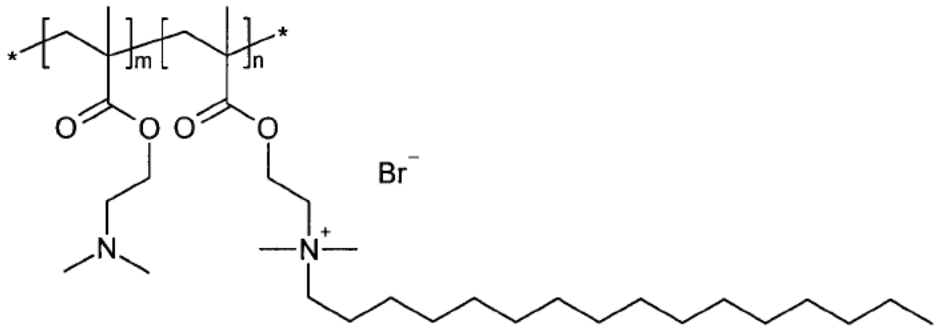
PMN:	P-04-0463	CAS RN:	88677-76-3

Chemical Name:
2-Propenoic acid, 2-methyl-, 2-(dimethylamino)ethyl ester, homopolymer, compd. with 1-bromohexadecane

Analogs:

Production Volume:

Structure:



95% 5%

Jullet (PMN)

Use: Thickener used in oil-field down hole application.
Analogs P-03-0315 and P-03-0316 are used as oil-field production aids. They increase the ratio of crude oil to produced water. They are injected into the underground oil-producing formation where they adhere to the rock. The presence of the polymers in the rock fissures allow the oil to pass, but retard the passage of water. This improves the efficiency of the oil well and reduces the amount of waste water that must be separated and

Formula:	$C_{32}H_{63}BrN_2O_4$	Eq Wt: 157 ⇒ 8.92% a-N (worst case)	
Mol Weight:	>100,000 ~~619.77~~	Wt%<500: 0.50	Wt%<1000 0.50
MP:		BP:	VP: <0.000001
H2O Sol (g/L):	Complete MSDS <0.000001	Physical State: Solid	Log P:

Endpoint (mg/L)	Est. Value	Meas. Value	Comments
Fish 96-h	0.28		
Daphnid 48-h	0.10		
Algal 96-h	0.040		
Fish ChV	0.016		
Daphnid ChV	0.007		
Algal ChV	0.020		
BCF			

CHEMICAL CLASS:

SAR: polymer – CAT – Q – N –

ECOTOX CONCERN (H) M L

CONCERN CONCENTRATION

DATE 4/2/04

ASSESSOR: